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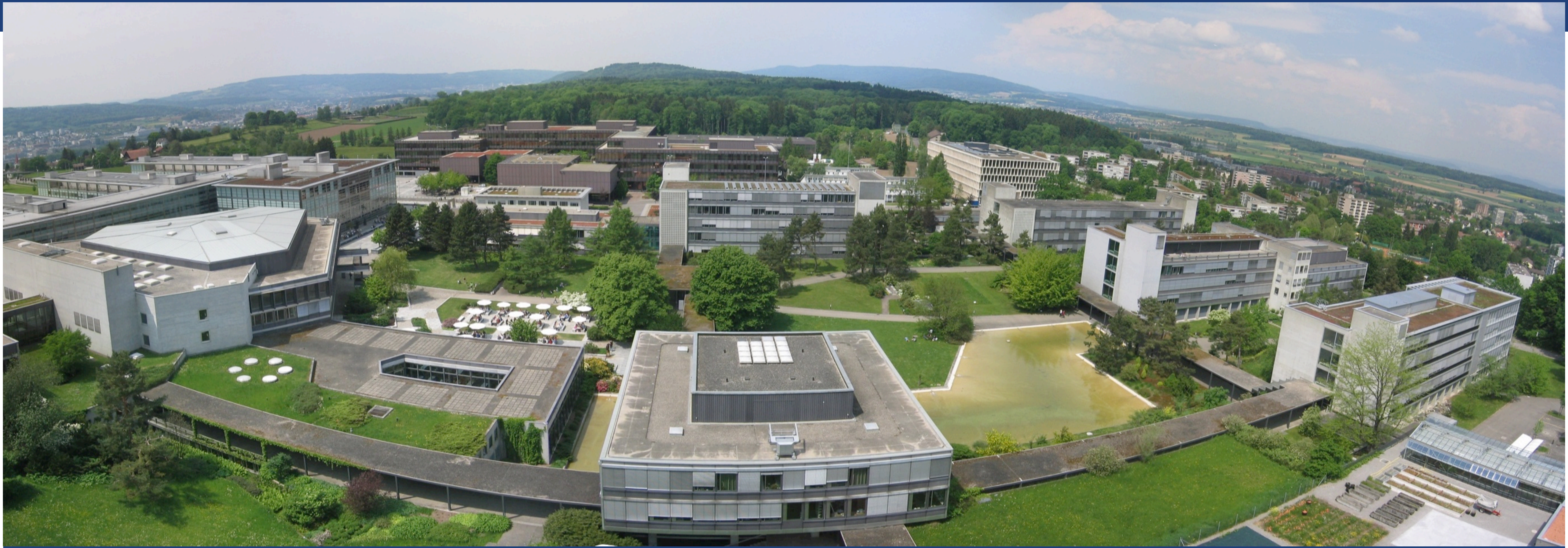

Case Studies in Process Design II

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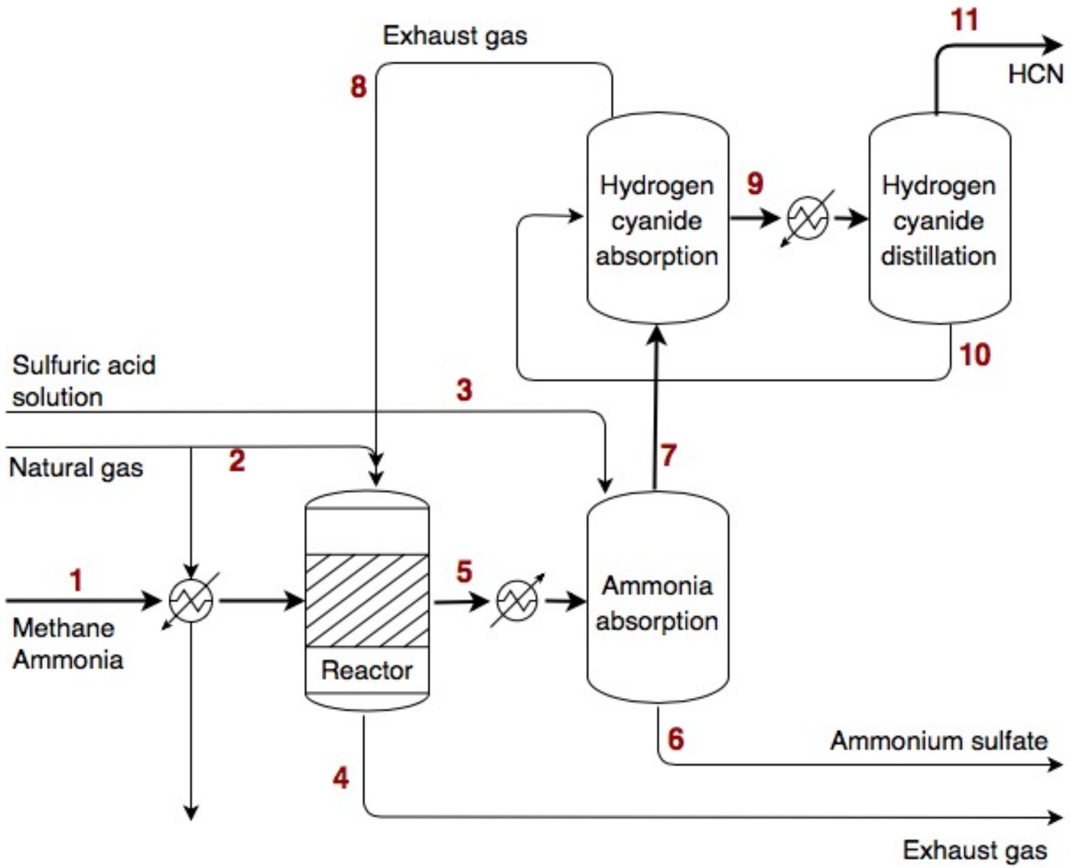


Reactor flow sheet

General Modelling Approach

- Four cases considered:

	Case 1	Case 2	Case 3	Case 4
Gas model	ideal gas law	ideal gas law	Peng-Robinson-EOS	Peng-Robinson-EOS
Heating mode	cross-current	cross-current	cross-current	co-current
Absorbers	shortcut model	shortcut model	non-ideal Eq.-model	non-ideal Eq.-model
Distillation	Fenske-Underwood-Gilliland	Fenske-Underwood-Gilliland	NRTL	NRTL
ΔP considered	no	yes	yes	yes

- Overall optimization with a “black box” approach

ODE-system governing the reactor

$$\frac{\mathrm{d}F_{\mathrm{N_2}}}{\mathrm{d}V} = r_2$$

$$\frac{\mathrm{d}F_{\mathrm{CH_4}}}{\mathrm{d}V} = -r_1$$

$$\frac{\mathrm{d}F_{\mathrm{NH_3}}}{\mathrm{d}V} = -r_1 - 2 \cdot r_2$$

$$\frac{\mathrm{d}F_{\mathrm{H_2}}}{\mathrm{d}V} = 3 \cdot r_1 + 3 \cdot r_2$$

$$\frac{\mathrm{d}F_{\mathrm{HCN}}}{\mathrm{d}V} = r_1$$

$$\frac{\mathrm{d}T}{\mathrm{d}V} = \frac{a \cdot U \cdot (T_a - T) - (r_1 \cdot \Delta H_{R_1} + r_2 \cdot \Delta H_{R_2})}{\sum_i F_i \cdot c_{p,i}}$$

$$\frac{\mathrm{d}T_a}{\mathrm{d}V} = \begin{cases} \frac{a \cdot U \cdot (T - T_a)}{\dot{m}_{Flu-Gas} \cdot c_{p,Flu-Gas}} & \text{for co-current heating} \\ 0 & \text{for cross-current heating} \end{cases}$$

$$\frac{\mathrm{d}P}{\mathrm{d}V} = \begin{cases} \frac{32 \cdot f_f \cdot \rho_{in} \cdot Q_{in} \cdot Q}{4 \cdot D^3} & \text{for considering a pressure drop} \\ 0 & \text{without pressure drop} \end{cases}$$

Assumptions for Ammonia Absorber

General

- Isothermal column
- Instantaneous & irreversible reaction
- Heat of absorption neglected
- Outlet temperature for liquid and gas alike
- No HCN absorption in water
- No pressure drop
- 20 % excess of sulfuric acid

Ideal case

- Heat capacities are T independent

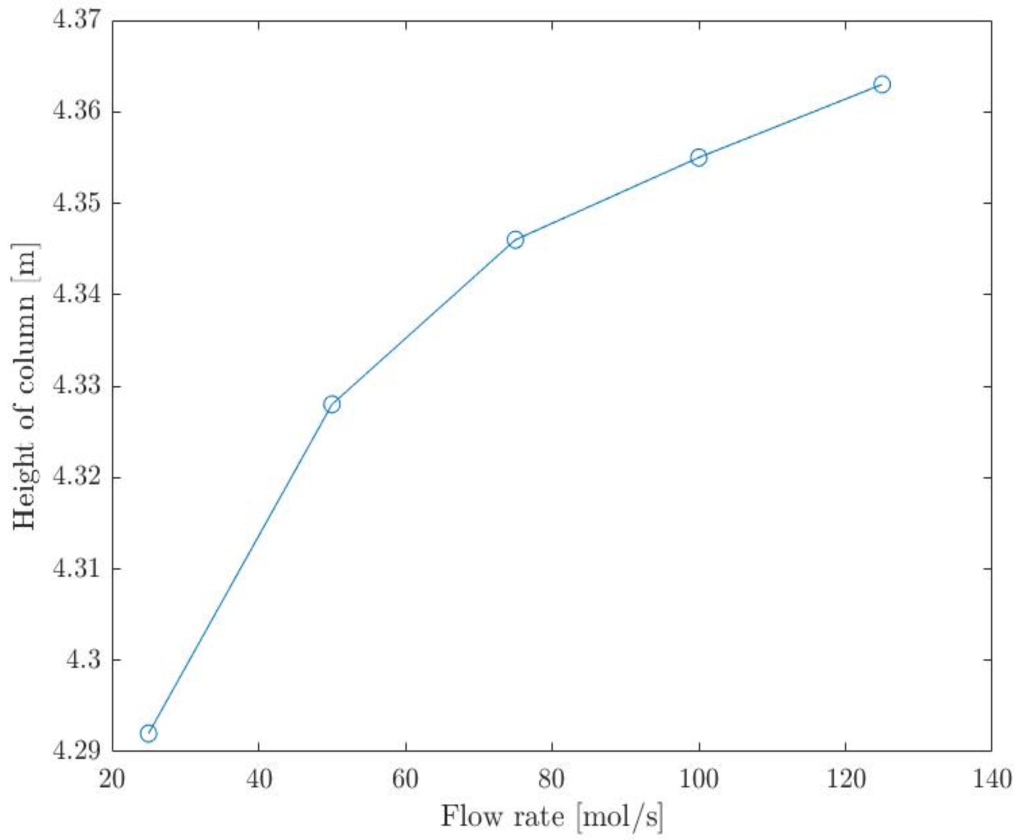
$$\Delta_f H(T) = \Delta_f H^0 + c_p \cdot (T - T_0),$$

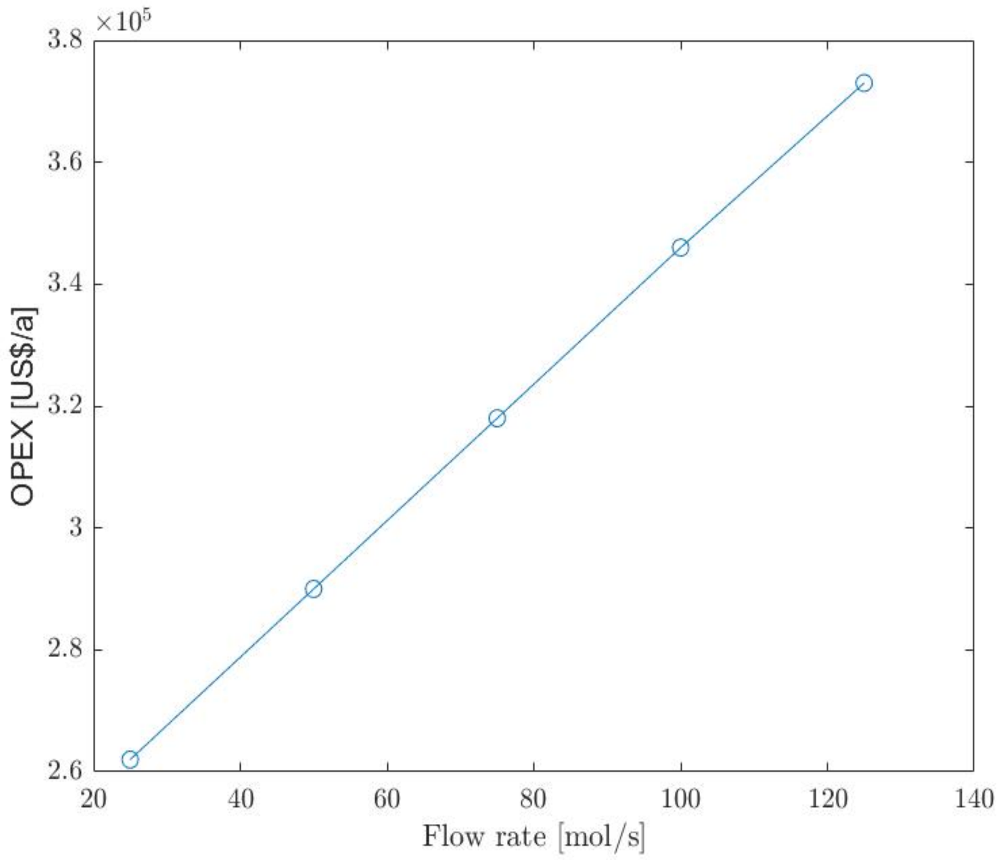
Non ideal case

- Heat capacities are T dependent

$$\Delta_f H_i(t) = \Delta_f H_i^0 + \left(A_i \cdot t + \frac{B_i \cdot t^2}{2} + \frac{C_i \cdot t^3}{3} + \frac{D_i \cdot t^4}{4} - \frac{E_i}{t} + F_i - H_i \right)$$

Sensitivity Analysis of the Ammonia Absorber





Made assumptions for the HCN absorber

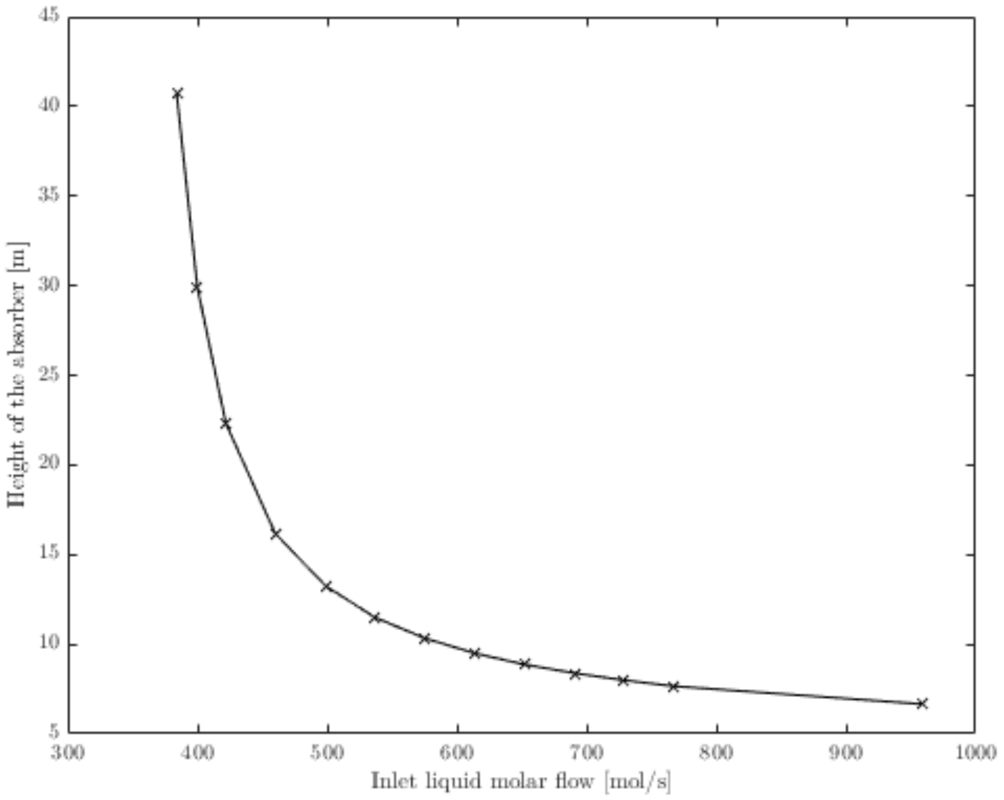
Ideal case

- Isothermal column
- Heat of absorption neglected
- Outlet temperature same for gas and liquid
- Only HCN is absorbed
- Heat capacities not temperature dependent
- No HCN in liquid inlet stream
- Resistivity in the liquid phase neglected

Non-ideal case

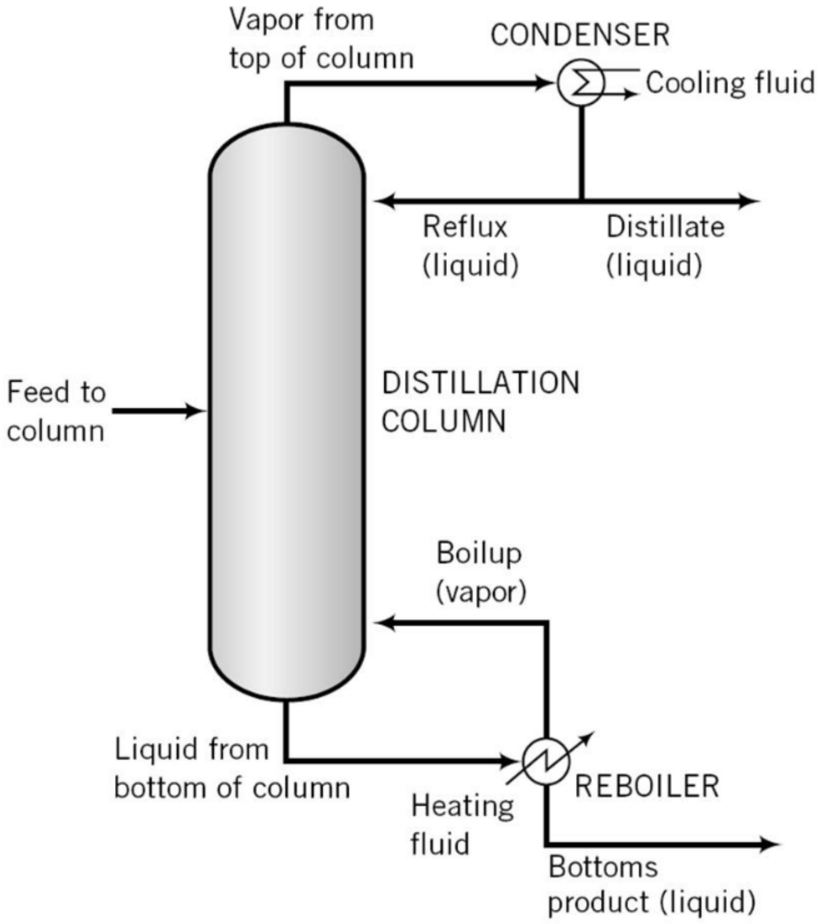
- Isothermal column
- Heat of absorption neglected
- Outlet temperature same for gas and liquid
- Only HCN is absorbed

Sensitivity analysis of the HCN Absorber



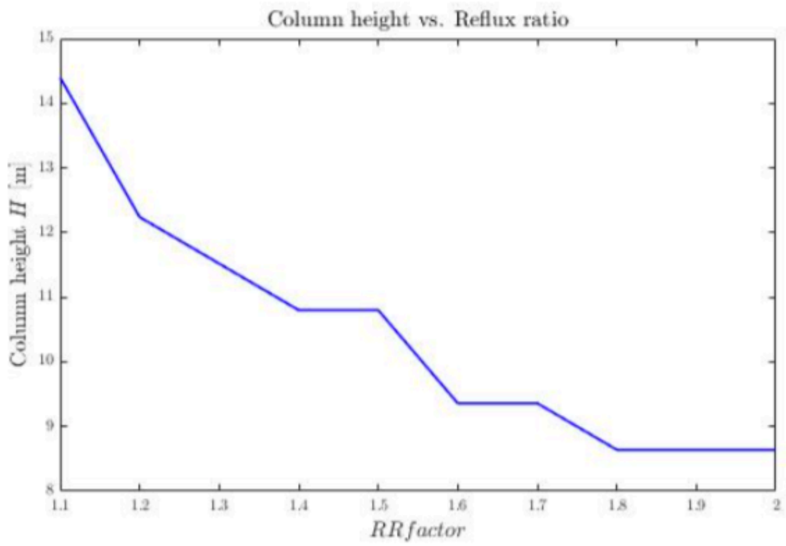
- Height of the column increases with decreasing inlet liquid flow
- Better absorption
- CAPEX decreases
- OPEX increases

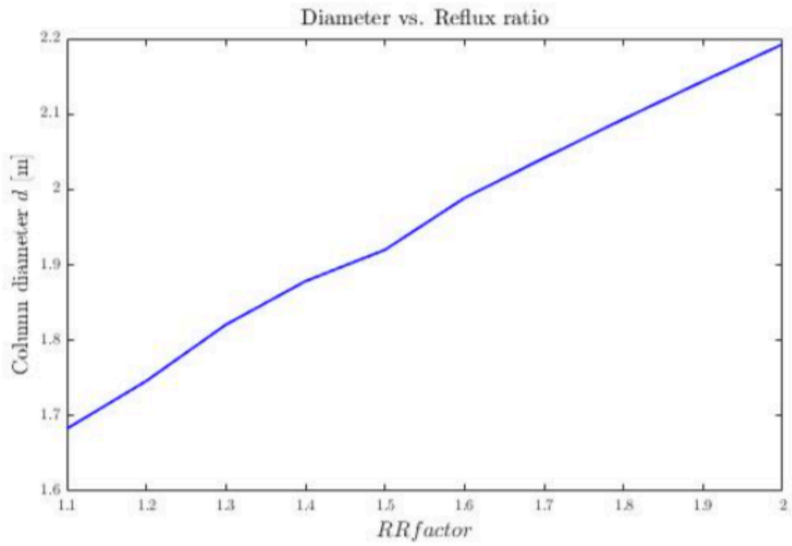
HCN Distillation

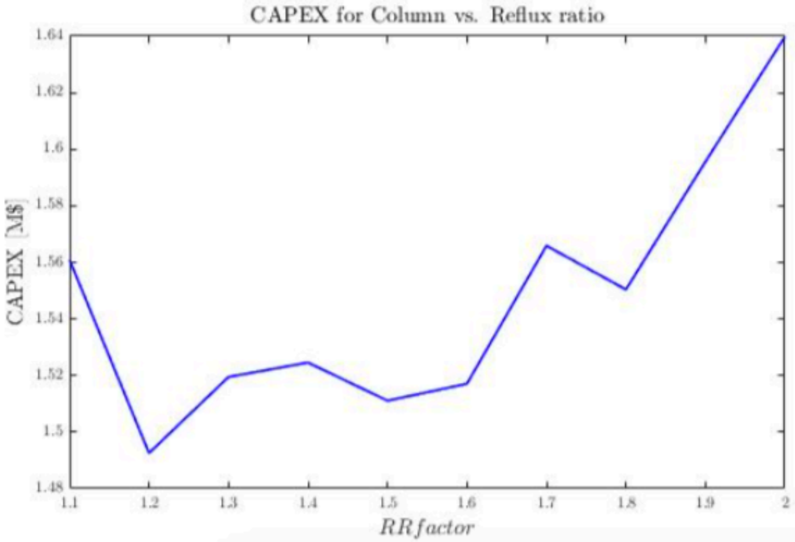


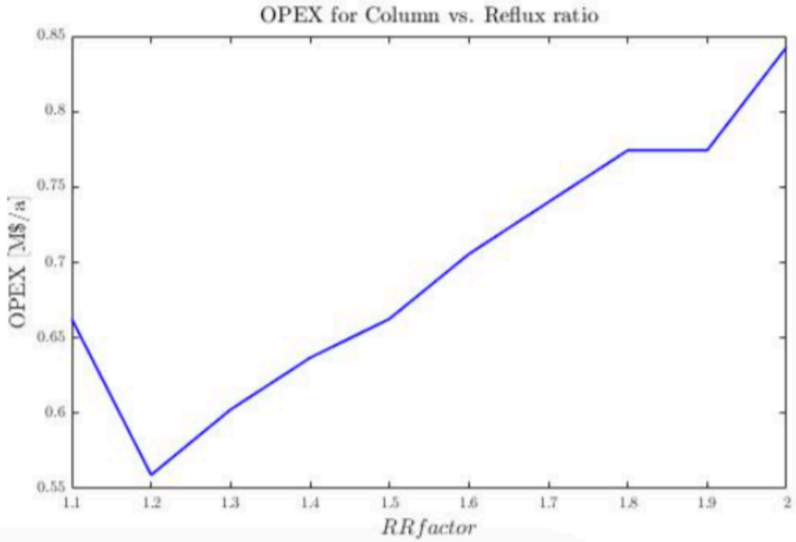
- Ideal or non-ideal (NRTL for liquid phase)
- No ΔP / ΔP
- Fenkse-Underwood-Gilliland method (justified since relative volatilities were pretty similar)
- x_{HCN}^{D} = 0.995, x_{HCN}^{B} = 10 ppm (going below these limits only makes the separation more difficult → higher CAPEX/OPEX)
- total condenser, q = 1 (requires another heat exchanger before the distillation column)

HCN Distillation









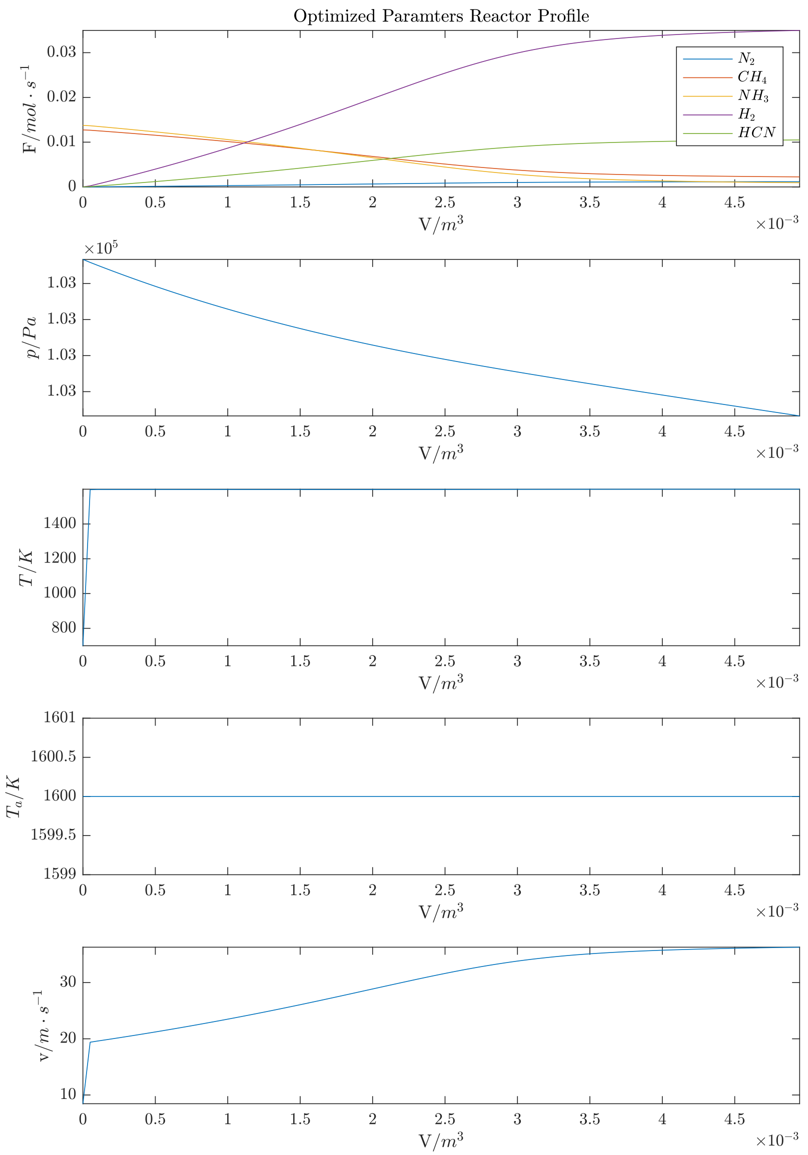
Results

Reactor:

- Ideal vs. real (case 1/case 3)
  - Length: 12 m / 28 m
  - Number of tubes: 1’342 / 17’149

- Cross- vs. co-current (case 3/case 4)
  - Number of tubes: 17’149 / 40’642
  - Heating medium flow: 0.10 / 0.05
  - Conversion CH_4: 0.82 / 0.59

Reactor profile case 3



Results

NH_3 absorber:

- Ideal vs. real (case 1/case 3)
  - Column height: 2.44 m / 4.39 m
  - Diameter: 0.79 m / 0.79 m
  - Flow rate ratio 0.80 / 1.64
  - Temperature in the column
  - Volumetric fraction H_2SO_4 : 0.37 / 2.01

Results

HCN absorber:

- Ideal vs. real (case 1/case 3)
  - Column height: 9.73 m / 10.31 m
  - Diameter: 1.11 m / 1.10 m
  - Outlet temperature: 294.72 K / 293.57 K
  - Water

Results

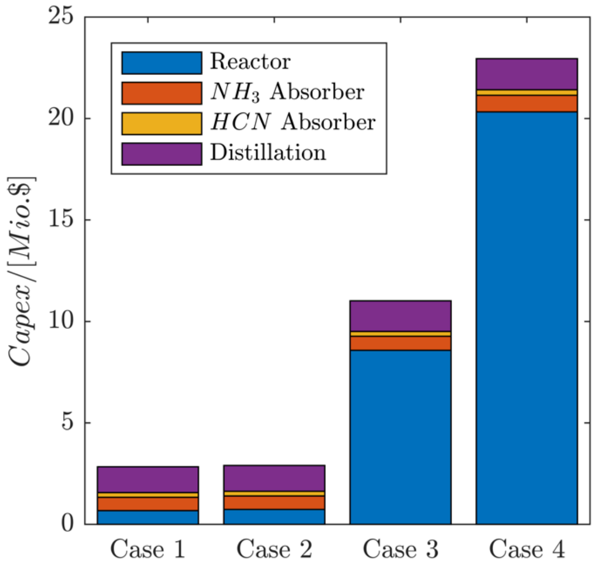
HCN distillation:

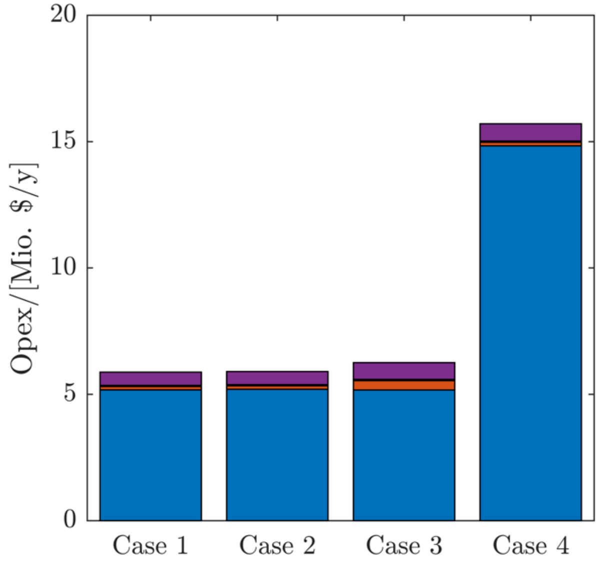
- Ideal vs. real (case 1/case 3)
  - Column height: 9.36 m / 10.08 m
  - Diameter: 1.73 m / 1.92 m
  - Heat exchanger area: 0.057 m^2 / 0.056 m^2

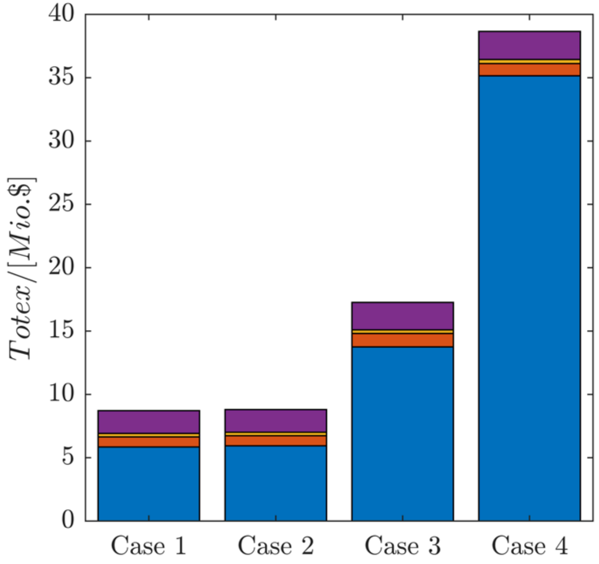
Results

Costs

- Ideal vs. real (case 1/case 3)
  - Break-even price: 0.62 \$/kg / 0.76 \$/kg







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Thank you for your attention